Comment on "Measurement of x-ray absorption spectra of overdoped high-temperature cuprate superconductors: Inapplicability of the single-band Hubbard model"

In a recent Letter, Peets, et al.[1] measured the x-ray intensity at the oxygen K-edge (hereafter referred to as LESW) in overdoped $La_{2-x}Sr_xCuO_{4\pm\delta}$ (LSCO) and $Tl_2Ba_2CuO_{6+\delta}$. They concluded that, unlike the underdoped samples of LSCO and $YBa_2Cu_3O_x$ in which LESW increases at least linearly[2] with doping, it saturates (see dashed lines in Fig. (1)c) abruptly for a hole count exceeding $x_c \approx 0.23$. They interpreted[1] the saturation as a breakdown of the 1-band Hubbard model in the cuprates. We analyse their data and show that this conclusion does not follow necessarily.

To clarify, the 1-band Hubbard model is designed to capture the low-energy features of the cuprates, particularly on the pseudogap scale. In fact, as demonstrated previously[3], beyond an energy scale of 500meV, deviations with the physics of the 3-band model are noticeable[3]. The oxygen K-edge experiments measure the unoccupied part of the density of states projected onto the oxygen 2p states. Hence, the relevant question is, can the 1-band Hubbard model reproduce the purported saturation with a cutoff on the integrated density of states of no more than 500meV? Indeed it can as shown in Fig. (1a). Shown here is a calculation of the integrated density of states using the dynamical cluster approximation (DCA), with a quantum Monte Carlo algorithm as the cluster solver[4]. We used a 16-site cluster. The densities of states produced by this method all show pseudogaps for the low-doping regime. Focusing entirely on the low-energy PG physics, we integrated the density of states up to a cutoff of $2J$. The calculations are for the lowest accessible temperatures, but the main feature that the integrated intensity levels once the pseudogap closes ($x = 0.13$ for $U = 6t$ and $x = 0.22$ for $U = 8t$) persists up to $T \sim J$ as is seen experimentally[1]. This is not an accident. When the pseudogap closes, Fermi liquid behaviour ensues, making it meaningless to separate the spectrum above the chemical potential into high and low energy parts.

Fig. (1a) is entirely **illustrative** because of course, **no** saturation obtains in the 1-band Hubbard model[5–7] if the cutoff encompasses the full LESW. But is the choice of the cutoff (and hence the purported deviation from the full weight in the 1-band model) relevant to the experiments? Fig. (1b) shows that it is not because regardless of the cutoff used to determine the LESW for LSCO, the saturation persists. Hence, the purported saturation in the experiments, if it truly exists, is unrelated to any high-energy scale. In fact, the width of integration with a cutoff of $528.5eV$ is identical to the integration range in the artificial calculation in Fig. (1a).

Nonetheless, it is difficult to reconcile a saturation of the full LESW with any known model. To investigate

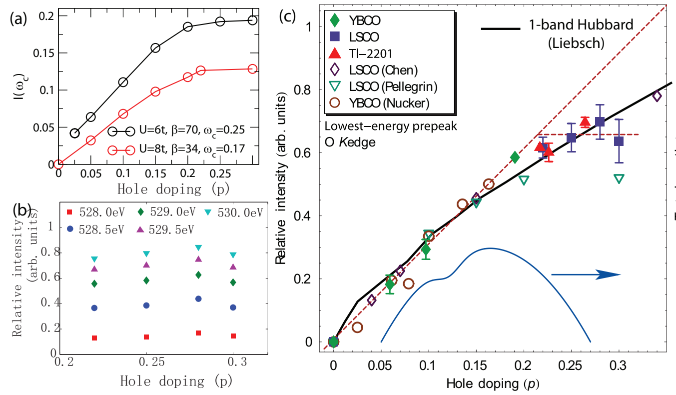

FIG. 1. a) Integrated densities of states on the interval $[0, \omega_c]$, for $U = 8t$ and $U = 6t$. b) Integrated oxygen K-edge intensity of the data of Peets, et al.[1] for LSCO with the cutoffs shown explicitly. c) Fig. (2) of Peets, et al.[1] overlayed (solid line) with the simulation data (Fig. 2a of Liebsch[7]) on the 1-band Hubbard model with an appropriately chosen y-axis scale factor to account for the mismatch with the units used in the experimental data. The dashed lines are due to Peets, et al.[1].

how robust the claim of saturation is, we overlay the recent cluster data (solid line in Fig. (1c)) of Liebsch[7] of the LESW evaluated with a doping-dependent cutoff that excludes any contribution from the upper band. The agreement with the data points (error bars included) is excellent. The slope change in the LESW in the 1-band Hubbard model reflects the fact that the dynamical spectral weight transfer[5, 6] (the explicit t/U corrections which make the LESW per spin exceed the doping level, x) must diminish above a certain doping level so that the non-interacting value of one state per site per spin is recovered at $n = 0$. Consequently, the claim that the experimental data (with error bars) imply a failure of the 1-band Hubbard model is not substantiated.

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